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Synchrotron Radiation and Photoelectron Group

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Research activities

I. Studies of electronic structures of solids and surfaces with X-ray and resonant photoemission[1-4]

(1) A photoemission study of ultrathin uranium layers on noble metals
(S. Fujimori, Y. Saito, T. Ejima, N. Sato, T. Komatsubara, S. Kunii, S. Suzuki, S. Sato, and T. Ishii)

The core levels and valence states of ultrathin uranium layers on gold and nickel substrates have been studied using XPS. Uranium coverage was less than 2.8 Å which corresponds to less than one monolayer. The spectral features are very similar to those of intermetallic compounds of uranium and gold or nickel. This indicates intermixing of deposited uranium with the substrates, at room temperature. In both U/Au and U/Ni systems, the main lines of U 4*f* spectra are quite asymmetric, and exhibit satellites at higher binding energies compared to the main lines. The profiles of the satellites are different in U/Au and U/Ni, reflecting the difference of the hybridization between U 5*f* and valence electrons of substrates.

(2) Correlation effect in resonant photoemission spectra of UPd_2Al_3 and UC
(T. Ejima, S. Sato, S. Suzuki, S. Fujimori, M. Yamada, N. Sato, Y. Onuki, T, Komatsubara, Y. Tezuka, S. Shin, and T. Ishii)

Both U5*f* partial density of states (DOS) and partial DOS without U5*f* for UPd_2Al_3 and UC were experimentally obtained by using U5*d*-5*f* resonant photoemission technique. Both spectra are compared with the results obtained by the energy band calculation. From the comparison, the spectra of U5*f* partial DOS cannot be reproduced by the band calculation except for the Fermi edge structures. In contrast, the spectra of partial DOS without U5*f* states are reproduced well by those from ligands. Those facts suggest that the spectra are not explained only by the band theory , but the correlation effect.

(3) Core level dependence of tailing structures in resonant spectra of UC and UB_{12}
(T. Ejima, S. Sato, S. Suzuki, S. Fujimori, M. Yamada, M. Kasaya, Y. Onuki, Y. Tezuka, S. Shin and T. Ishii)

Two kinds of difference spectra of UC and UB_{12} are obtained through U5$d_{5/2}$-and U5$d_{3/2}$-5*f* resonant processes. In the spectra, spectral intensity of the satellite structure around 3 eV varies as the excited ptoton energy changes. This tendency leads to the speculation that the differences in 5*f* fhotoemission spectrum under off-resonance and various on-resonance conditions arise from differences in selection rules as is proposed in 4*f* spectrum.

(4) Photoemission and ion scattering study of Ce/Ni(110) and Ce/Cu(110) systems
(T. Okane, M. Yamada, S. Suzuki, S. Sato, Toyohiko Kinoshita, A. Kakizaki, T. Ishii, T. Kobayashi, S. Shimoda, M. Iwaki, and M. Aono)

We have studied the electronic structures of Ce/Ni(110) and Ce/Cu(110) systems by the 4*d*→4*f* resonant photoemission using synchrotron radiation and the Ce 3*d* core-level x-ray photoemission. We also investigated the distribution of component atoms in surface layers of Ce/Ni(110) system by the medium-energy ion scattering. In Ce/Ni(110) system, strength of the hybridization between 4*f* and conduction electrons (*f*-c hybridization) significantly depends on the Ce concentration in the surface layers. In Ce/Cu(110) system, the *f*-c hybridization is very weak and insensitive to the Ce concentration in the surface layers.

II. Design and instrumentation for synchrotron radiation facility[5-7]

(5) Lattice design of a synchrotron radiation source at Tohoku University
(M. Katoh, S. Sato, S. Suzuki, and T. Yamakawa)

A 1.5 GeV strage ring was designed for a synchrotron radiation facility planned at Tohoku University. A stretcher-booster ring, which is now under construction, will be used as an injector. The circumference of the ring is 187 m. The beams emittance is 7 nm-rad. The ring consists of 12 double bend achromatic cells. Ten of 12 dispersion-free long straight sections are 5m long and will be used for insertion devices, RF cavities and injection. Other two are 15m long and reserved for advanced devices such as a very long undulater or a free electron laser. The present status of the project is 'waiting for approval'.

(6) A profilometer for Synchrotron Radiation Mirrors
(S. Sato, T. Mori, Y. Higashi, S. Haya, M. Otsuka, and H. Yamamoto)

A profilometer for measuring surface figures of large-size aspheric mirrors was constructed on the basis of the Twyman-Green interferometer with heterodyne phase detection method. By using overlapping mesurement method, surface profiles of a cylindrical mirror 1000 mm length were evaluated within the designed accuracy.

(7) Aspherically bent SiC mirror : Bending test
(E. Ishiguro, H. Sugawara, M. Okuyama, N. Waku, S. Sato, and T. Takigawa)
A bending test of an elliptically bent SiC mirror was performed. The result shows that a desired figure of the surface can be generated with a high accuracy by using a simple bending mechanism.

III. High-resolution photoemission study of high-Tc superconductors and related compounds[8-19),32)]

(8) High-resolution angle-resolved photoemission study of non-cuprate two-dimensional superconductor Sr_2RuO_4
(T. Yokoya, O. Akaki, H. Kumigashira, A. Chainani, T. Takahashi, H. Katayama-Yoshida, M. Kasai and Y. Tokura)
High-resolution angle-resolved photoemission spectroscopy has been carried out on a ruthenate superconductor Sr_2RuO_4 (Tc = 1 K) which has the same crystal structure as La_2CuO_4, but with RuO_2 layers replacing the CuO_2 , and exhibits T^2 dependence of electrical resistivity below 25 K. The results show that the electronic structure of Sr_2RuO_4 has an extended van-Hove singularity (VHS) near E_F in a quite similar manner to the high Tc cuprates, regardless of the character of the electronic states near E_F. This requests reexamination of the VHS scenario and its relation to both the normal and superconducting properties.

(9) Extended van-Hove singularity in a non cuprate layered superconductor Sr_2RuO_4
(T. Yokoya, A. Chainani, T. Takahashi, H. Katayama-Yoshida, M. Kasai and Y. Tokura)
Angle-resolved photoemission spectroscopy was performed on a ruthenate superconductor Sr_2RuO_4 (Tc = 0.93 K) which has the same crystal structure as La_2CuO_4, but with RuO_2 layers replacing CuO_2, and exhibits T^2 dependence of resistivity. We found that Sr_2RuO_4 has an extended van-Hove singularity (VHS) close to E_F like high Tc cuprates, regardless of the character of the electronic states at E_F. This suggests that the extended VHS is a general feature of a two-dimensional *d*-electron metal. The observed Fermi surface is in contrast to local-density-approximation calculations.

(10) Extended van-Hove singularity in Sr_2RuO_4 observed by angle-resolved photoemission
(T. Yokoya, A. Chainani, T. Takahashi, H. Katayama-Yoshida, M. Kasai, and Y. Tokura)
We have performed a low-temperature high-resolution angle-resolved photoemission spectroscopy on a non-cuprate superconductor Sr_2RuO_4 (Tc ~ 1 K) which has the same crystal structure as La_2CuO_4, but with RuO_2 layers replacing CuO_2. We found that Sr_2RuO_4 has an extended van-Hove singularity (VHS) close to E_F (20 ± 2 meV) like high-Tc cuprates, regardless of the character of the electronic states at E_F, suggesting that the extended VHS is a general feature of a two-dimensional *d* -electron metal. This requests re-examination of the VHS scenario for superconducting properties of cuprates, while for T-linear resistivity it seems to be consistent with this result.

(11) Evidence for Correlation Effects in Sr_2RuO_4 from Resonant and X-ray Photoemission Spectroacopy
(T. Yokoya, A. Chainani, T. Takahashi, H. Katayama-Yoshida, M. Kasai, Y. Tokura, N. Shanthi, and D. D. Sarma)
We study the electronic structure of Sr_2RuO_4, a non-cuprate layered superconductor (Tc = 0.93K) using electron spectroscopy. X-ray photoemission spectroscopy shows that the single particle occupied density of states(DOS) is in fair agreement with the calculated DOS. However,

resonant photoemission spectroscopy across the Ru 4p-4d threshold establishes the existence of a correlation satellite to the Ru 4d band. The results indicate substantial charge-transfer character at the Fermi level, with on-site correlations U_{dd} comparable in magnitude to the Ru-O hopping integral, like the cuprates.

(12) Electronic excitation in $Bi_2Sr_2CaCu_2O_8$: Fermi surface, dispersion, and absence of bilayer splitting

(H. Ding, A. F. Bellman, J. C. Campuzano, M. Randeria, M. R. Norman, T. Yokoya, T. Takahashi, H. Katayama-Yoshida, T. Mochiku, K. Kadowaki, G. Jennings, and G. P. Brivio)

From a detailed study, including polarization dependence, of the normal state angle-resolved photoemission spectra for $Bi_2Sr_2CaCu_2O_8$, we find only one CuO_2 band related feature. All other spectral features can be ascribed either to umklapps from the superlattice or to "shadow bands." Even though the dispersion of the peaks looks like band theory, the line shape is anomalously broad and no evidence is found for bilayer splitting. We argue that the "dip feature" in the spectrum below T_c arises not from bilayer splitting, but rather from many-body effects.

(13) Extended van-Hove singularity in non-cuprate perovskite superconductor Sr_2RuO_4

(T. Takahashi, T. Yokoya, A. Chainani, H. Katayama-Yoshida, M. Kasai, and Y. Tokura)

Low-temperature high-resolution angle-resolved photoemission spectroscopy (ARPES) have been performed on a non-cuprate superconductor Sr_2RuO_4 ($T_c \sim 1$ K), which has the same crystal structure as La_2CuO_4, but with RuO_2 layers replacing CuO_2. High-resolution ARPES spectra obtained along Γ - Z line (Ru-O bonding direction) in Brillouin zone show the existence of an extended van-Hove singularity (VHS) close to E_F (20 ± 2 meV) like high-T_c cuprates, regardless of the character of the electronic states at E_F, suggesting that an extended VHS is a general feature of correlated two-dimensional *d* - electron metals. This requests re-examination of the VHS scenario for superconducting properties of cuprates, while the observed T-linear resistivity seems to be consistent with the present result.

(14) High-resolutionangle-resolved photoemission spectroscopy of the momentum dependence of superconducting gap in $Bi_2Sr_2CaCu_2O_8$

(T. Yokoya, T. Takahashi, T. Mochiku, and K. Kadowaki)

The momentum dependence of the superconducting gap in $Bi_2Sr_2CaCu_2O_8$ has been studied using high-resolution angle-resolved photoemission spectroscopy (ARPES) with non-polarized light. The size of superconducting gap obtained at several points on the Fermi surface shows a linear dependence with respect to the gap function of $d_{x^2-y^2}$ wave defined as $0.5 \times |\cos k_x a - \cos k_y a|$. This suggests that the anomaly in the superconducting gap observed with polarized light is not intrinsic, being due to the superstructure of BiO plane, but that the strong anisotropy of superconducting gap like $d_{x^2-y^2}$ symmetry is intrinsic.

(15) Direct observation of particle-hole mixing in the superconducting state by angle-resolved photoemission

(J. C. Campuzano, H. Ding, M. R. Norman, M. Randeria, A. F. Bellman, T. Yokoya, T. Takahashi, H. Katayama-Yoshida, T. Mochiku, and K. Kadowaki)

Particle-hole (*p-h*) mixing is a fundamental consequece of the existence of a pair condensate. We present direct experimental evidence for *p-h* mixing in the angle-resolved photoemission (ARPES) spectra in the superconducting state of $Bi_2Sr_2CaCu_2O_{8+\delta}$. In addition to its pedagogical importance, this establishes unambiguously that gap observed in ARPES is associated with superconductivity.

(16) Spectroscopic evidence for a pseudogap in the normal state of underdoped high-Tc superconductors

(H. Ding, T. Yokoya, J. C. Campuzano, T. Takahashi, M. Randeria, M. R. Norman, T. Mochiku, K. Kadowaki, and J. Giapintzakis)

It is well known that BCD means-field theory is remarkably successful in describing conventional superconductors. A central concept of BCS theory is the energy gap in the electronic excitation spectrum below the superconducting transition temperature, T_c. The gap also serves as the order parameter: quite generally, long-range phase coherence and a non-zero gap go hand-in-band. But in underdoped high-T_c superconductors there is considerable evidence that a pseudogap (a suppression of spectral weight) is already formed in the normal state above T_c first, from studies of the spin excitation spectrum[2-5,24], which measure a 'spin gap', and later from a variety of other probes[6-10]. Here we present a study of underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) using angle-resolved photoemission spectroscopy (ARPES), which directly measures the momentum-resolved electron excitation spectrum of the CuO_2 planes. We find that a pseudogap with *d*-wave symmetry opens up in the normal state below a temperature $T^* > T_c$, and develops into the *d*-wave superconducting gap once phase coherence is established below T_c.

(17) Angle-resolved photoemission study of Sr_2RuO_4

(T. Yokoya, A. Chainani, T. Takahashi, H. Ding, J. C. Campuzano, H. Katayama-Yoshida, M. Kasai, and Y. Tokura)

We present high-resolution (HR) angle-resolved photoemission spectroscopy (ARPES) measurements of the non-cuprate layered perovskite superconductor Sr2RuO4. ARPES spectra of the whole valence-band region obtained along two high symmetry directions in the Brillouin zone show clear dispersion, generally similar to that of a band calculation. However, HRARPES measurements taken in the vicinity of the Fermi level (E_F) show narrower Ru4dε(xy,yz,zx)-O2pπ anti-bonding bands than those predicted by the band calculation. More significantly, there is an extended van Hove singularity very close to E_F (E_B = 11 meV) along the Ru-O bonding direction, which is known to exist in cuprate high temperature superconductors. The Fermi-surface topology obtained by HRARPES (one electron-like Fermi surface sheet centered at the Γ point and two hole-like sheets centered at the X point) is different from the band calculation (two electron-like sheets centered at the Γ point and one hole-like sheet centered at the X point), although the electron count is the same in both cases. These results suggest that electron-electron correlations cause the modification of the Fermi-surface topology, and is thus necessary for understanding the electronic structure and properties of Sr2RuO4.

(18) Angle-resolved photoemission spectroscopy study of the superconducting gap anisotropy in $Bi_2Sr_2CaCu_2O_{8+x}$

(H. Ding, M. R. Norman, J. C. Campuzano, M. Randeria, A. F. Bellman, T. Yokoya, T. Takahashi, T. Mochiku, and K. Kadowaki)

We report measurements of the momentum dependence of the superconducting gap in $Bi_2Sr_2CaCu_2O_{8+x}$ with angle-resolved photoemission spectroscopy using a dence sampling of the Brillouin zone in the vicinity of the Fermi surface. In the *Y* quadrant of the zone, where there are no complications from ghost bands caused by the superlattice, we find a gap function consistent within error bars to the form $\cos(k_x)-\cos(k_y)$ expected for a *d*-wave order parameter. Similar results are found in the *X* quadrant with the photon polarization chozen to enhance main band emission over that due to ghost bands.

(19) Evolution of the Fermi surface with carrier concentration in $Bi_2Sr_2CaCu_2O_{8+\delta}$

(H. Ding, M. R. Norman, J. C. Campuzano, M. Randeria, T. Takeuchi, T. Yokoya, T. Takahashi, T. Mochiku, and K. Kadowaki)

We show, by use of angle-resolved photoemission spectroscopy, that underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ appears to have a large Fermi surface centered at (π, π), even for samples with a T_c as low as 15K. No clear evidence of a Fermi surface pocket around $(\pi/2, \pi/2)$ has been found. These conclusions are based on a determination of the minimum gap locus in the pseudogap regime $T_c<T<T^*$, which is found to coincide with the locus of gapless excitations in momentum space (Fermi surface) determined above T^*. These results suggest that the pseudogap is more likely of precursor pairing rather than magnetic origin.

IV. High-resolution photoemission study of f-electron materials[20-24]

(20) High-resolution photoemission study of UNi_2Al_3 and URu_2Si_2

(S.-H. Yang, H. Kumigashira, T. Yokoya, A. chainani, N. Sato, T. Komatsubara, S.-J. Oh, and T. Takahashi)

High-resolution low-temperature photoemission spectroscopy has been performed for UNi_2Al_3 and URu_2Si_2 to study the nature of 5f electrons in U-based heavy fermion materials. Photoemission spectra of both compounds have a sharp peak at E_F and a large broad peak around 2 eV, while only UNi_2Al_3 exhibits an additional small broad feature at 0.6 eV. The two features in the vicinity of E_F (the E_F-peak and the small structure at 0.6 eV) are found to have a dominant U 5f character while the prominent peak around 2 eV is due to the Ni 3d or Ru 4d states. Comparison with the band structure calculations and experimental results on UPd_2Al_3 suggests that the E_F-peak is ascribed to itinerant U 5f electrons while the following broad feature at 0.6 eV represents localized f electrons.

(21) High-resolution photoemission study of $CeRu_2$; the dual character of 4f electrons

(S.-H. Yang, H. Kumigashira, T. Yokoya, A. Chainani, T. Takahashi, H. Takeya, and K. Kadowaki)

High-resolution low-temperature photoemission spectroscopy was performed for $CeRu_2$ to study the nature of low-lying excitations around the Fermi level (E_F). It was found that the photoemission spectrum near E_F shows well-resolved two peaks at and about 270 meV below E_F, which are ascribed to the tail of the Ce $4f1$ final state located just above E_F and its spin-orbit satellite ($\Delta SO \sim 270$ meV), respectively. This suggests that the many-body correlation effect is necessary for understanding the electronic structure near E_F of $CeRu_2$, although the Ce $4f$ electron exhibits a substantially itinerant character through the strong hybridization with the conduction electrons.

(22) High-Resolution Photoemission Study of UNi_2Al_3 and URu_2Si_2

(S.-H. Yang, H. Kumigashira, T. Yokoya, A. Cjainani, T. Takahashi, S.-J. Oh, N. Sato, and T. Komatsubara)

High-resolution low-temperature photoemission spectroscopy has been performed for UNi_2Al_3 and URu_2Si_2 to study the nature of $5f$ electrons in U-based heavy fermion materials. Photoemission spectra of both compounds have a sharp peak at E_F and a large broad peak around 2 eV, while only UNi_2Al_3 exhibits an additional small broad feature at 0.6 eV. The two features in the vicinity of E_F (the E_F-peak and the small structure at 0.6 eV) are found to have a dominant U $5f$ character while the prominent peak around 2 eV is due to the Ni $3d$ or Ru $4d$ states. Comparison with the band structure calculations and experimental results on UPd_2Al_3 suggests that the E_F-peak is ascribed to itinerant U $5f$ electrons while the following broad feature at 0.6 eV represents localized f electrons.

(23) High-resolution angle-resolved photoemission spectroscopy of CeBi

(H. Kumigashira, S.-H. Yang, T. Yokoya, A. Chainani, T. Takahashi, A. Uesawa, T. Suzuki, O.

Sakai, and Y. Kaneta)

High-resolution angle-resolved photoemission spectroscopy (HR-ARPES) has been performed on a CeBi single crystal to study the complicate electronic structure near the Fermi level (E_F). The experimental result was compared with the band structure calculation based on the p-f mixing model as well as the de-Haas van Alphen (dHvA) effect measurements. It was found that the overall feature of the valence band shows a remarkably good agreement between the experiment and the calculation, suggesting the essential validity of the p-f mixing model. HR-ARPES measurement near E_F has established the existence of a small electron pocket centered at M point in the Brillouin zone, supporting the band calculation and the dHvA measurement. HR-ARPES spectra around G point show some dispersive bands near EF indicative of a hole pocket centered at Γ point, though it was not so clearly resolved as the electron pocket due to close proximity of individual bands. These results are consistent with a semi-metallic nature of CeBi. The observed quantitative discrepancy between the experiment and the calculation is discussed.

(24) High-resolution angle-resolved photoemission study of CeP; Narrow-band formation of 4f electrons

(H. Kumigashira, S.-H. Yang, T. Yokoya, A. Chainani, T. Takahashi, A. Uesawa, and T. Suzuki)

High-resolution angle-resolved photoemission spectroscopy at low temperature has been performed on a low-carrier Kondo material CeP. It was found that the p-f bonding state with a dominant 4f character exhibits a finite energy dispersion of about 40 meV along the ΓX direction in the Brillouin zone. This implies that 4f electrons in CeP form a narrow band owing to the strong anisotropic p-f and d-f mixing.

V. High-resolution photoemission study of low-dimensional organic conductors[25-31]

(25) High-resolution photoemission study of deutrated dimethyl-dicyanoquinoinediimine-Cu compound; $(DMe\text{-}DCNQI)_2Cu$

(T. Takahashi, T. Yokoya, A. Chainani, A. Tanaka, H. Kumigashira, O. Akaki, and R. Kato)

High-resolution photoemission spectroscopy has been carried out for *in-situ* synthesized deutrated organic conductor $(DMe\text{-}DCNQI)_2Cu$, where DMe-DCNQI is dimethyl dicyano-quinonediimine, to study the metal-insulator transition due to the charge ordering. The high-resolution photoemission spectrum near EF shows a rigid shift of about 100 meV indicative of opening of a Peierls gap below the critical temperature (Tc= 60 K).

(26) Electron spectroscopic studies of the organic conductors DCNQI (N, N'-dicyanoquinonediimine)-Cu salts

(A. Tanaka, A. Chainani, T. Yokoya, T. Takahashi, T. Miyazaki, S. Hasegawa, and T. Mori)

We have carried out a comparative study of the electronic structure of *in-situ* synthesized quasi-one-dimentional organic conductors $(DMe\text{-}DCNQI)_2$ using various electron spectroscopic techniques (UPS , XPS , and AES), where DMe-DCNQI and MeBr-DCNQI are From these results we discussed the differences in electronic stuructures between two salts that lead to their different electrical and magnetic properties.

(27) Electronic structure of the quasi-one-dimensional halogen-bridged Ni complexes $[Ni(chxn)_2X]X_2$(X=Cl, Br) and related Ni compounds

(H. Okamoto, Y. Shimada, Y. Oka, A. Chainani, T. Takahashi, H. Kitazawa, T. Mitani, K. Totiumi, K. Inoue, T. Manabe, and M. Yamashita)

The electronic structure of the one-dimensional Ni complexs, $[Ni(chxn)_2X]X_2$(*X*=Cl, Br; (chxn)=1*R*, 2*R*-cyclohexanediamine), is studied together with the discrete Ni complexes,

[NiX_2([14]aneN$_4$)]ClO_4 (X=Cl; Br; ([14]aneN$_4$) = 1,4,8,11-tetraazacyclotetradecane), using optical spectroscopy, x-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy. The optical spectra show that the Br compounds have a smaller gap as compared with the Cl compounds. An analysis using a simple X-Ni-X trimer model on the optical spectra and the Ni 2p XP spectra yields quantitative estimates for the charge transfer (CT) energy Δ and the transfer energy T for discrete and one-dimensional Ni complexes. The analysis on the Ni LVV Auger spectra in conjunction with the valence XP spectra indicates that the average on-side d-d Coulomb energy U in the one-dimensional and discrete Ni complexes is about 5 eV, quite similar to the case of the Ni dihalides. The obtained results demonstrate that the one-demensional Ni complexes are CT insulators. We discuss the differences in the electronic structures of the one-dimensional Ni complexes compared with the Ni dihalides and the one-dimensional Pt complexes on the one-dimensional Pt complexes on the basis of the estimated parameter values of Δ, T, and U.

VI. Photoemission study of fullerens[28-29]

(28) Photoemission study of K- and Sc-doped C_{84}

(A. Ito, O. Akaki, and T. Takahashi)

The electronic structure of solid C_{84} with doping of K or Sc metal was studied by ultraviolet photoemission spectroscopy. Successive filling of the LUMO (lowest unoccupied molecular orbital), LUMO+1, and LUMO+2 bands by electrons donated from doped K atoms was clearly observed in K-doped C_{84}. In the case of Sc-doped one, no clear successive filling of unoccupied bands was observed although new electronic states appear between the HOMO (highest occupied molecular orbital) band and the Fermi level with doping. In either of K- and Sc-doped solid C_{84}, no clear Fermi-edge cutoff indicative of its metallic nature was observed in the spectrum.

(29) Electronic structures of C_{70} crystalline phases

(K. Ohno, J.-Z. Yu, Y. Maruyama, Y. Kawazoe, and T. Takahashi)

By means of an all-electron mixed basis approach, band structures of the C_{70} crystalline phases are calculated for the first time for fcc, hcp(c/a = 1.633) and also sc structures with at most four molecules inside a unit cell. The resulting densites of states are compared with our photoemission and inverse photoemission data of C_{70} powder study and the best agreement between the experiment and the present theory is found the hcp symmetry.

VII. High-resolution photoemision study of various interesting materials (magnetite and gold)[30-31]

(30) Electronic structure of Fe_3O_4 across the Verwey transition

(A. Chainani, T. Yokoya, T. Morimoto, T. Takahashi, and S. Todo)

A study of the first-order Verwey transition in single-crystal Fe_3O_4 using high-resolution temperature dependent (100-300K) photoemission spectroscopy is reported. Fe_3O_4 exhibits a gap of 70~meV in the occupied part of the density of states (DOS) below the transition temperature, T_v=122K. On increasing the temperature above T_v, the gap in the DOS is closed thus establishing a metal-semiconductor transition. The Fe 3d derived features arising from $Fe^{3+}(eg^2)$ majority and Fe^{2+} (t_{2g}^1) minority spin states responsible for the transition, retain their character just above the transition but merge into a single feature by 300K. Simultaneously, the DOS at E_F increases systematically in the metallic phase. The results indicate a gradual change in the short- range order for $T > T_v$ which gives rise to the non-metallic like electrical conductivity observed just above T_v.

(31) High-resolution temperature-dependent valence band photoemission spectroscopy of gold: Nature of electron-phonon coupling
(T. Yokoya, A. Chainani, and T. Takahashi)

Using high-resolution temperature-dependent (20 - 400 K) *valence-band* photoemission spectroscopy, we study the nature of electron-phonon coupling in polycrystalline gold. The valence band shows systematic broadening for increasing temperatures which is well-reproduced by a Gaussian broadening of the 20 K spectrum. It depends linearly on temperature and is found to be excessive (~9 kBT). The results suggest the existence of anharmonic lattice vibrations and a quadratic electron-phonon coupling, similar to the case of aluminum 2p core-levels.

Doctor Theses

(1) Han-Woong Yeom (June, 1996)
Structure and electronic properties of adsorbates on the Si(001) surface studied by photoelectron-diffraction and-spectroscopy

(2) Takayoshi Yokoya (March, 1997)
Construction of High-Resolution Photoemission Spectrometer and Study of Superconducting Gap of Bi-High-Tc Superconductors

Master Theses (March, 1997)

(1) Osamu Akaki
Photoemission Spectroscopy of Low-Dimensional Organic Conductor DCNQI-Metal Compounds

(2) Hiroshi Kumigashira
High-Resolution Photoemission Study of Cerium Compounds

(3) Kazutoshi Takahashi
Photoemission study of quantum size effects on metal nanofilms

(4) Koji Tamura
Photoemission study of single-crystal rare-earth hexaborides

(5) Munenori Mizuta
Study of unocuppied states in rare-earth compounds by using an inverse photoemission spectrometer of the energy dispersive type

Publications

(1) Aphtoemission study of ultrathin uranium layers on noble metals,
S. Fujimori, Y. Saito, T. Ejima, N. Sato, T. Komatsubara, S. Kunii, S. Suzuki, S.Sato, and T. Ishii
J. Electron Spectroscopy and Related Penomena **78** (1996) 155-158.

(2) Correlation effect in resonant photoemission spectra of UPd_2Al_3 and UC,
T. Ejima, S. Sato, S. Suzuki, S. Fujimori, M. Yamada, N. Sato, Y. Onuki, T. Komatsubara,

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